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Phonon interaction of electrons in the translation-invariant strong-coupling theory

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A dependence of phonon interaction on the interelectronic distance is found for a translation-invariant (TI) strong-coupling bipolaron. It is shown that the charge induced by the electrons in a TI-bipolaron state is always greater than that in a bipolaron with spontaneously broken symmetry.

Keywords: Froehlich Hamiltonian; polaron; correlation length; Coulomb; quark.

Considerable attention given to the bipolaron problem in recent years centers around attempts to explain the superconductivity phenomenon with the use of the mechanism of Bose-condensation of bipolaron gas^{1,2,3}. In this context the study of the interaction between the electrons caused by their interaction with phonons is a vital task. In papers^{4–6} a new concept of a translation-invariant bipolaron (TI-bipolaron) was introduced which possesses much higher coupling energy, than a bipolaron with spontaneously broken symmetry (SBS-bipolaron). Of interest is to calculate the interaction energy as a function of a distance between the electrons in a TI-bipolaron and to find the value of the charge induced by the electrons in a polar medium. Notice that for the case of SBS-bipolarons, these points were discussed in a lot of papers^{7–9}. Following^{4–6}, we will proceed from Froehlich Hamiltonian for a bipolaron which in the coordinates of the center of mass has the form:

$$\hat{H} = -\frac{\hbar^2}{2M_e}\Delta_R - \frac{\hbar^2}{2\mu_e}\Delta_r + U(|\vec{r}|) + \sum_k \hbar\omega_k a_k^+ a_k + \sum_k 2 \cos \frac{\vec{k}\vec{r}}{2} \left(V_k e^{i\vec{k}\vec{R}} a_k + H.C. \right) \quad (1)$$

where R , r are coordinates of the center of mass and relative motion of electrons, respectively: $M_e = 2m$, $\mu_e = m/2$, m is an electron mass, a_k^+ , a_k are operators of a phonon field; $V_k = (e/k)\sqrt{2\pi\hbar\omega/\tilde{\epsilon}V}$, $\tilde{\epsilon}^{-1} = \epsilon_\infty^{-1} - \epsilon_0^{-1}$, $\omega_k = \omega$ is a phonon frequency, e is an electron charge, ϵ_∞^{-1} , ϵ_0^{-1} are high-frequency and static dielectric constants, V is the systems volume, $U(r) = e^2/\epsilon_\infty |\vec{r}|$.

After excluding the center of mass coordinate by means of Heisenberg transformation¹⁰, with the use of Lee-Low-Pines transformation (LLP)¹¹:

$$S_2 = \exp \left\{ \sum_k f_k (a_k - a_k^+) \right\}, \quad (2)$$

2 *Lakhno V.D.*

the energy of electron-phonon interaction of the electrons $U_{int}(r)$, according to (1), is written as:

$$U_{int}(r) = \left\langle 0 \left| S_2^{-1} \left(\sum_k 2V_k \cos \frac{\vec{k}\vec{r}}{2} (a_k + a_k^\dagger) \right) S_2 \right| 0 \right\rangle = 4 \sum_k V_k f_k \cos \frac{\vec{k}\vec{r}}{2}. \quad (3)$$

According to ⁶, when the LLP function f_k is chosen in the Gaussian form:

$$f_k = -N\vec{V}_k \exp(-k^2/2\mu),$$

$$\vec{V}_k = 2V_k \left\langle \Psi \left| \cos \frac{\vec{k}\vec{r}}{2} \right| \Psi \right\rangle, \Psi(r) = \left(\frac{2}{\pi l^2} \right)^{3/4} \exp(-r^2/l^2), \quad (4)$$

where N, μ, l are varying parameters, with the use of (3) $U_{int}(r)$ is expressed as:

$$\tilde{U}_{int}(\tilde{r}) = -\sqrt{\frac{x^2 + 16y}{x^2 + 8y}} \frac{1}{\tilde{r}} F\left(\frac{2\tilde{r}}{\sqrt{16y + x^2}}\right), F(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt, \quad (5)$$

where $\tilde{U}_{int}(\tilde{r}) = U_{int}(r)/(4me^4/\hbar^2\tilde{\epsilon}^2)$, $\tilde{r} = (e^2m/\hbar^2\tilde{\epsilon})r$ - are dimensionless variables. The values of $x = x(\eta)$, $y = y(\eta)$ (where $\eta = \epsilon_\infty/\epsilon_0$ is the parameter of ion coupling) for each η value are determined from the condition that the function $\Phi(x, y; \eta)$ be minimum ⁶:

$$\Phi(x, y; \eta) = \frac{6}{x^2} + \frac{20, 25}{x^2 + 16y} - \frac{16\sqrt{x^2 + 16y}}{\sqrt{\pi}(x^2 + 8y)} + 4\frac{\sqrt{2/\pi}}{x(1 - \eta)}. \quad (6)$$

Relation of quantities x, y with the parameters μ, l in (4) is given by formulae $x = l\alpha$, $y = \alpha^2/\mu$, where:

$$\alpha = (e^2/\hbar\tilde{\epsilon}) \sqrt{m/2\hbar\omega}, \quad (7)$$

is a constant of electron-phonon coupling.

Fig.1 demonstrates the dependencies $\tilde{U}_{int}(\tilde{r})$ for some values of η parameter. It is seen that for small \tilde{r} , the interaction potential is independent of \tilde{r} , for intermediary has linear dependence on r , while for large \tilde{r} , it has a Coulomb form: $\tilde{U}_{int}(\tilde{r}) \sim 1/\tilde{r}$. Fig.1 also suggests that at the point $\eta = \eta_c = 0,289$, i.e. at the point where a TI-bipolaron decays into TI-polarons ⁶, interaction $U_{int}(r)$ does not demonstrate any jumps and changes continuously as η increases up to the value of $\eta = 1 - 1/2\sqrt{2}$, at which the total energy of a TI-bipolaron $E_{bp} = \Phi\alpha^2$ vanishes. The total interaction potential $U_{tot}(r)$ should include the Coulomb interaction $U(r)$:

$$U_{tot}(r) = U_{int}(r) + U(r), \quad (8)$$

and is shown on Fig. 1 (upper solid curve).

It looks like Coulomb interaction in the case of small r and has a near-linear shape in a certain range of r variation (this is especially clear in fig.1 f): $\eta = 0,6$). This behavior reminds the interaction between quarks, with repulsive instead attractive

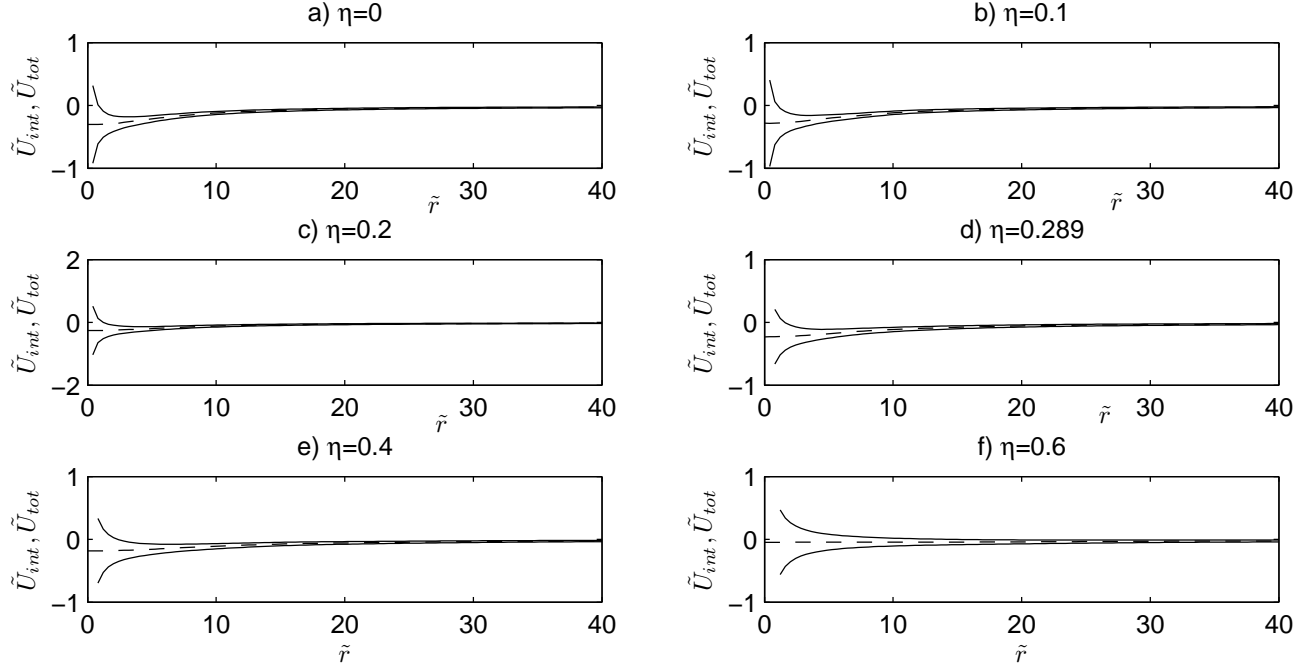


Fig. 1. The dependence of interaction potentials \tilde{U}_{int} (dashed), total potential \tilde{U}_{tot} with positive $U(r)$ in (8), which corresponds to electron Coulomb repulsion (upper solid curve) and negative $U(r)$ (lower solid curve) which corresponds to quark attraction, on η .

as in the case of quark Coulomb potential (Fig. 1, lower solid curve). (A polaron model of quarks was considered in ¹²).

The knowledge of $U_{int}(r)$ enables us to calculate the density distribution of a charge $\rho_{ind}(r)$ induced by electrons in a polar medium. Assuming:

$$U_{int}(r) = -2e\varphi_{ind}(r), \quad (9)$$

where $\varphi_{ind}(r)$ is a potential induced by the electrons, we will write for $\rho_{ind}(r)$:

$$\Delta_r \varphi_{ind}(r) = 4\pi \rho_{ind}(r). \quad (10)$$

With the use of (5), (9), (10) we express $\rho_{ind}(r)$ as:

$$\rho_{ind}(r) = \frac{32}{\pi} \sqrt{\frac{2}{\pi}} \frac{e}{\epsilon} \left(\frac{me^2}{\hbar^2 \tilde{\epsilon}} \right)^3 \tilde{\rho}(\tilde{r})$$

$$\tilde{\rho}(\tilde{r}) = \frac{1}{(x^2 + 16y)\sqrt{x^2 + 8y}} \exp(-8\tilde{r}/(16y + x^2)). \quad (11)$$

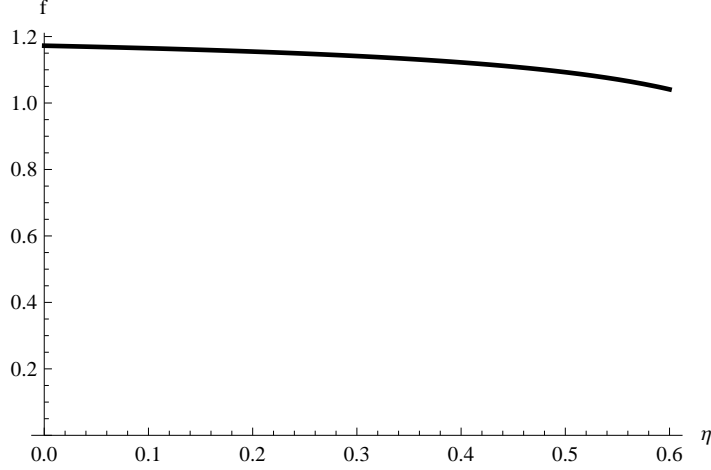
4 *Lakhno V.D.*

Fig. 2. The dependence of function $f = \sqrt{(16y + x^2)/(8y + x^2)}$ on η

The total charge Q induced by a TI-bipolaron:

$$Q = \int \rho_{ind}(r) dV, \quad (12)$$

is equal to:

$$Q = \sqrt{\frac{16y + x^2}{8y + x^2}} \frac{2e}{\tilde{\epsilon}}. \quad (13)$$

Fig.2 shows the dependence of $f = \sqrt{(16y + x^2)/(8y + x^2)}$ as a function of the parameter η . Fig.2 suggests that the value of a charge Q induced by the electrons in a TI-bipolaron state is always greater than that of a charge $2e/\tilde{\epsilon}$ induced by the electrons in a SBS-bipolaron state. These values coincide only for $\eta \rightarrow 1 - 1/2\sqrt{2}$ - value, when the effective distance between the electrons in a TI-bipolaron (correlation length) is equal to infinity. This result suggests that the adiabatic approximation in this limit holds for a TI-polaron too.

In conclusion it may be said that the frequently introduced concept of inter-polaronic interaction^{2,7-9} in the case of a TI-bipolaron is objectless, since even for large r , a TI-bipolaron cannot be presented as the one consisting of two individual polarons (here an analogy with confinement of quarks is appropriate).

This presentation, however, can be sensible, if for a certain value ($\eta = \eta_c$) a decay of a TI-bipolaron into two individual TI-polarons is possible. For this case, the dependence of the polarons interaction on the distance was calculated in⁹.

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